Quality Technology & Quantitative Management
Vol. 2, No. 2, pp. 147-160, 2005

QTQM

Computer-Generated Experimental Designs for Irregular-Shaped Regions

Nam-Ky Nguyen[1] and Greg F. Piepel[2]

[1]School of Mathematics, Statistics and Computer Science,
University of New England, Armidale, NSW, Australia
[2]Statistical Sciences, Battelle-Pacific Northwest
Division, Richland, Washington, USA
(*Received* March 2004, *accepted* February 2005)

Abstract: This paper focuses on the construction of computer-generated designs on irregularly-shaped, constrained regions. Overviews of the Fedorov exchange algorithm (FEA) and other exchange algorithms for the construction of D-optimal designs are given. A faster implementation of the FEA is presented, which is referred to as fast-FEA (denoted FFEA). The FFEA was applied to construct D-optimal designs for several published examples with constrained experimental regions. Designs resulting from the FFEA are more D-efficient than published designs, and provide benchmarks for future comparisons of design construction algorithms. The construction of G-optimal designs for constrained regions is also discussed and illustrated with a published example.

Keywords: ACED, DETMAX, D-optimality, Fedorov exchange algorithm, genetic algorithm, G-optimality, mixture experiment, optimal designs.

1. Introduction

Standard statistical designs (e.g. factorial, fractional factorial, Plackett-Burman, central composite, and Box-Behnken) are widely used in many scientific and industrial studies. However, such designs are generally only applicable to experimental regions that can be scaled to cubes or spheres, and have other limitations. Hence, they may not applicable in many situations, in which case computer-generated designs (CGDs) are often used. Montgomery [11] and Montgomery *et al.* [12] (hereafter MLJT) mentioned three situations in which they deemed CGDs appropriate:

(i) An irregular-shaped experimental region: In this situation, the experimental region is subject to constraints, such as for constrained mixture experiment designs.

(ii) A nonstandard model: There are cases in which experimenters may be led by their knowledge of the process being investigated to use models other than those supported by standard designs.

(iii) Unusual sample size requirements: The amount of experimental material, or the time or budget available for conducting an experiment, may not correspond to the numbers of design points in standard designs. Instead of using a smaller standard design with the number of points satisfying experimental limitations, experimenters might prefer to use a more flexible CGD with a number of points closer to that allowed by the experimental budget.

CGDs are commonly generated using point-exchange algorithms (PEAs) to select design points from a candidate set so as to optimize a design criterion (a mathematical measure of design *goodness*). The most popular design criterion is D-optimality, which involves selecting a design matrix X to minimize $|\mathrm{X}'\mathrm{X}|^{-1}$. Other design criteria are discussed in a subsequent section. Although not widely available in experimental design software, no-candidate-set algorithms, such as coordinate-exchange algorithms (CEAs) and genetic algorithms (GAs), also are available for generating CGDs. Algorithms for generating CGDs are discussed more in a subsequent section.

This paper focuses on constructing CGDs for irregular-shaped experimental regions. Two recent papers on this subject are MLJT (to which we have already alluded) and Heredia-Langner *et al.* [6] (hereafter HCMBR). The latter paper used several real examples involving constrained regions to demonstrate that a GA can produce D-optimal designs as good or better than PEAs. This paper is intended as a sequel to MLJT and HCMBR and has the following objectives:

(i) To explain the optimal design problem, review the Fedorov exchange algorithm (FEA) and other PEAs, and advocate a faster implementation of the FEA for the construction of D-optimal experimental designs. This implementation is referred to as fast-FEA, and denoted FFEA.

(ii) To show that the FFEA runs very quickly and generates designs with improved values of optimality criteria compared to published designs for several examples.

(iii) To set benchmarks for comparing algorithms for constructing D-optimal designs involving the success rate in producing the best designs and the time used to construct these designs.

(iv) To show that the FFEA for D-optimal designs can be used to generate G-optimal designs and that these designs are comparable to those generated by the generalized DETMAX algorithm for G-optimal designs discussed by Welch [21] and implemented in ACED (Welch [22]).

An outline of the rest of the paper is as follows. Section 2 discusses the optimal design problem and several optimality criteria. Section 3 proposes an approach for obtaining G-optimal designs from D-optimal designs. Section 4 discusses the FEA and other PEAs, which may be considered as approximations of the FEA. Section 5 discusses alterations to the FEA's implementation, yielding the FFEA that greatly reduces the computational time. Section 6 discusses the designs obtained applying the FFEA to several examples from the literature and compares the properties of the resulting designs to those published in the literature. Section 7 provides some concluding remarks.

2. The Optimal Design Problem and Optimality Criteria

The optimal design problem can be defined as choosing an n-point design to optimize a specified design criterion. Several popular design criteria (also referred to as optimality criteria) are discussed in the subsequent paragraph. The traditional approach used to solve an optimal design problem involves selecting the n design points from a candidate set S of N points. However, some no-candidate-set approaches have been presented in the literature, as mentioned in the Introduction.

The linear model for m factors (or components in the case of mixture experiments) in n runs in matrix notation is $E(\boldsymbol{y}) = \mathrm{X}\boldsymbol{\beta}$, where $\boldsymbol{y}$ is an $n \times 1$ vector of observations,

$\mathbf{X}$ is an $n \times p$ matrix of model terms ($p \geq m$) that contains n row vectors of model terms $\mathbf{x}_i'$ (obtained from the design point x_i), and $\boldsymbol{\beta}$ is a $p \times 1$ vector of model regression coefficients. Assuming that $\mathbf{X}'\mathbf{X}$ is nonsingular, several common optimality criteria involve minimizing various functions of $(\mathbf{X}'\mathbf{X})^{-1}$:

(i) D-optimality: Minimizing $|\mathbf{X}'\mathbf{X}|^{-1}$ (or maximizing $|\mathbf{X}'\mathbf{X}|$) results in minimizing the generalized variance of the estimated coefficients and minimizing the volume of the confidence ellipsoid of $\boldsymbol{\beta}$ (assuming the errors are normally distributed).

(ii) A-optimality: Minimizing trace $(\mathbf{X}'\mathbf{X})^{-1}$ results in minimizing the average variance of the estimated coefficients.

(iii) G-optimality: Minimizing $v_{\max} = \max\{v_i\}$ results in minimizing the maximum standardized prediction variance, where $v_i = \mathbf{x}_i'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_i$ is the prediction variance standardized by σ^2. Ideally, $v_{\max}$ should be calculated over the entire experimental region. However, many design generation software that rely on a set of candidate points only calculate $v_{\max}$ over the set of candidate points.

(iv) V-optimality: Minimizing $\bar{v} = \text{avg}\{v_i\}$ results in minimizing the average standardized prediction variance. Again, ideally $\bar{v}$ should be calculated over the entire experimental region, but many design generation software only calculate $\bar{v}$ over the set of candidate points.

Note that all of the preceding criteria involve the matrix X, which is referred to as the *model* matrix because it expands the design matrix according to the assumed model form.

3. D-Optimality as a Criterion for Constructing G-Optimal Designs

The D-optimality criterion has been more popular than other optimality criteria because of computational advantages. Welch [21] argued that the heavy focus on D-optimality is inappropriate, because in practice many experiments are aimed at estimating the response over the region of interest rather than parameter estimation. He therefore generalized Mitchell's DETMAX algorithm (Mitchell [8]) to implement G- (and V-) optimality in his ACED program (Welch [22]). However, he mentioned two frustrations in implementing the G-optimality criterion: (i) G-optimality is expensive (i.e., computationally intensive and time consuming) and (ii) the G-optimality criterion is prone to getting trapped in local optima, and hence does not necessarily produce designs with higher G-efficiency than the D- (or V-) optimality criterion. G-efficiency is defined as $100p/(nv_{\max})$.

Although D- and G-optimality are not necessarily equivalent for n-point designs, a design that is good with respect to the D-optimality criterion is generally also good with respect to the other optimality criteria. Some classical designs such as the 2^m factorials and Plackett-Burman designs are in fact D-, A-, G-, and V-optimal. Nguyen and Miller [16] used this observation to produce 2^m fractional factorial designs of resolution V with high A-efficiency, for $7 \leq m \leq 10$ and for various values of n by selecting the best A-optimal design out of a large pool of generated D-optimal designs. Over years of using both the D- and G-optimality criteria in ACED to construct constrained mixture designs, the second author has often observed that the design with the best G-efficiency often results from one of the tries with the D-optimality criterion.

Based on the preceding discussion, we propose obtaining a G-optimal design by selecting the best G-optimal design among a large number of designs produced by the D-optimality criterion. This approach is illustrated in Example 5 of Section 6. There are three advantages of this approach to constructing G-optimal designs: (i) D-optimality requires less computation and time than G-optimality, (ii) D-optimality is not necessarily sacrificed at the cost of G-optimality, and (iii) it is easier to implement a D-optimality algorithm than a G-optimality algorithm. However, this approach may fail if there is little variation in the quality of the D-optimal designs produced.

4. The Fedorov Exchange Algorithm and its Approximations

Nearly all design generation software use at least one form of PEA. Critical to all PEAs are updating formulas that simplify the matrix calculations involved in the calculating the optimality criteria previously discussed. Let $\mathrm{M} = \mathrm{X}'\mathrm{X}$, where X is as previously discussed. If x' (a row vector obtained from the design point x) is to be augmented to or removed from X, we have:

$$| \mathrm{M} \pm \mathrm{x}\mathrm{x}' | = | \mathrm{M} | \, (1 \pm \mathrm{x}'\mathrm{M}^{-1}\mathrm{x}), \tag{1}$$

$$(\mathrm{M} \pm \mathrm{x}\mathrm{x}')^{-1} = \mathrm{M}^{-1} \mp \mathrm{u}\mathrm{u}' / (1 \pm \mathrm{x}'\mathrm{M}^{-1}\mathrm{x}), \tag{2}$$

where $\mathrm{u} = \mathrm{M}^{-1}\mathrm{x}$. Now if x' is to be augmented to X and x_i' (a row vector obtained from the design point x_i) is to be removed from X simultaneously, we have:

$$| \mathrm{M} + \mathrm{x}\mathrm{x}' - \mathrm{x}_i\mathrm{x}_i' | = | \mathrm{M} | \, \{1 \pm \Delta(x_i, x)\}, \tag{3}$$

where $\Delta(x_i, x) = \mathrm{x}'\mathrm{M}^{-1}\mathrm{x} - \mathrm{x}_i'\mathrm{M}^{-1}\mathrm{x}_i + (\mathrm{x}'\mathrm{M}^{-1}\mathrm{x}_i)^2 - \mathrm{x}'\mathrm{M}^{-1}\mathrm{x}\mathrm{x}_i'\mathrm{M}^{-1}\mathrm{x}_i$. (4)

The quantity $\Delta(x_i, x)$ is often referred to as Fedorov's delta function.

The FEA and comparisons of the FEA performance with other PEAs are discussed in detail by Cook and Nachtsheim [1], Nguyen and Miller [15], and Miller and Nguyen [7]. Here we briefly discuss the FEA (considered as the most computationally expensive PEA). The FEA, developed by Fedorov [2, 3], consists of the following steps:

Step 1: Start with a randomly chosen non-singular n-point design. Compute M, $|\mathrm{M}|$ and M^{-1};

Step 2: Find simultaneously a point x_i in the current n-point design and a point x in S (the candidate set) such that $\Delta(x_i, x)$ calculated by Equation (4) is maximum and exchange x_i with x. Update $|\mathrm{M}|$ and M^{-1} using Equations (2) and (3).

Step 2 is repeated until $\Delta(x_i, x)$ is less than ε, a chosen small positive number.

As previously noted, the FEA is a very expensive algorithm. Consider the mixture problem with one process variable in HCMBR (see Example 2 of Section 6) where 15 runs are selected from a candidate set of 273 points (a 273-point grid). There are 4095 ($=15 \times 273$) delta functions to evaluate in each iteration and only one result of these 4095 evaluations is ever used. Hence, there have been several attempts to modify or approximate the FEA.

The Wynn-Mitchell algorithm due to Mitchell and Miller [10] and Wynn [23] breaks each iteration (i.e., each step (ii) of the FEA) into two stages. At the first stage, a point x in S is found such that $\mathrm{x}'\mathrm{M}^{-1}\mathrm{x}$ is maximum and then x is added to the current n-point design. At the second stage, a point x_i in the $(n+1)$-point design is found such that $\mathrm{x}_i'\mathrm{M}^{-1}\mathrm{x}_i$ is minimum, and x_i is removed to yield an n-point design. The DETMAX algorithm of Mitchell [8] generalizes this PEA to permit *excursions* in the sense that at each iteration, t (instead of 1) points can be added to (or removed from) the design.

The modified FEA (MFEA) of Cook and Nachtsheim [1] broke each iteration of the FEA into n stages. At stage i $(i = 1,\ldots,n)$, point x_i in the n-point design is exchanged with a point x in S (x is a point which maximizes $\Delta(x_i, x)$). Cook and Nachtsheim [1] noted that their MFEA produces designs that are comparable to those produced by the FEA and is about twice as fast as the FEA. Due to this fact, the MFEA is used as a default PEA in several optimal design software packages.

5. A Fast Fedorov Exchange Algorithm

If we study the steps of the PEAs in the previous section in detail, it becomes clear that when a design is constructed by the FEA, it is impossible for an approximating algorithm (such as the Wynn-Mitchell algorithm or the MFEA) to improve it. However, when a design is constructed by an approximating algorithm, there is a possibility for the FEA to improve it. Unfortunately, the FEA in its original form might be prohibitively expensive to use (Cook and Nachtsheim [1]).

The following alterations to the implementation of the FEA to accelerate its performance are therefore proposed:

(i) For each try, use a partially random design instead of a completely random design as starting design (Galil and Kiefer [4]). For a partially random design, n_0 $(n_0 < n)$ points are randomly selected from N candidate points. Now a candidate point x_i is added to this n_0-point design if $\mathrm{x}_i'\mathrm{M}^{-1}\mathrm{x}_i$ is maximum and this process continues until n points are included in the starting design. Note that several tries are required to ensure a good design is obtained as any PEA can get trapped in local optima.

(ii) Update $\mathrm{x}_i'(\mathrm{M} \pm \mathrm{xx}')^{-1}\mathrm{x}_i$ from $\mathrm{x}_i'\mathrm{M}^{-1}\mathrm{x}_i$ instead of calculating the former afresh (Galil and Kiefer [4]).

(iii) Reduce the number of $\Delta(x_i, x)$'s to evaluate by evaluating only those whose sum of the first two terms in Equation (4) is greater than δ, the largest value of $\Delta(x_i, x)$ obtained at a particular point. Note that from the Cauchy-Schwarz inequality, the last two terms in Equation (4) will never be greater than 0 (Nguyen and Miller [15] and Miller and Nguyen [7]).

We refer to this faster implementation of the FEA as fast-FEA, which is denoted FFEA. The FFEA is used for all examples in the following section.

6. Examples

We now consider five examples from the literature in which computers were used to construct designs for constrained regions. We document the performance of the FFEA for each example, and show how it improves the published designs in terms of D-optimality (Examples 1-4) and G-optimality (Example 5).

6.1. Example 1: Adhesive Bond Strength Experiment

Montgomery [11] pp. 466-472 and MLJT presented an example in which the experimenter investigated the strength of an adhesive in joining two parts. The two factors of interest are: the amount of adhesive applied to the two parts (x_1) and the cure temperature (x_2). This example reappears in HCMBR with the following constraints for the coded values of these two factors $-1 \le x_i \le 1$ and $-0.5 \le x_1 + x_2 \le 1$. Figure 3 of HCMBR displays a 12-point design obtained by applying a GA to a 266-point grid. The candidate set contains those points on a grid of step size 0.1 that satisfy the mentioned constraints. A second-order polynomial in x_1 and x_2 was assumed, with the goal of generating a D-optimal design. The HCMBR 12-point design, listed in the first two columns of Table 1, has $|X'X|^{-1}$ = 3.545E-3.

We now show how the FFEA works by using these points as a starting design. In the first iteration, the FFEA replaces point (–1, 1) with point (0, 1) and reduces $|X'X|^{-1}$ to 3.240E-3. In the second iteration, the FFEA replaces point (0.5, –1) with point (–0.1, –0.4) and reduces $|X'X|^{-1}$ to 3.191E-3. In the third iteration, the FFEA replaces point (–1, 0.5) with point (1, –1) and reduces $|X'X|^{-1}$ to 3.114E-3. In the fourth iteration, the FFEA replaces point (–0.1, –0.4) with point (–0.2, –0.3). The resulting design (the last two columns in Table 1) has $|X'X|^{-1}$ =3.106E-3. These four iterations also reduce $v_{\max}$ of the HCMBR design from 0.8497 to 0.6754 and increase the G-efficiency from 58.9 to 74.0.

We gave FFEA the mentioned 266-point candidate set and 1000 tries to work on this same problem. The 1000 tries consumed 4 seconds on a 2GHz laptop running under Linux. Each try obtained a design with the same $|X'X|^{-1}$ =3.106E-3. Thus the average number of successes per second for this example is 250 (=1000/ 4). For this example, HCMBR reported a design obtained by the MFEA with $|X'X|^{-1}$ =3.696E-3. We suspect that HCMBR did not perform a sufficient number of tries with the MFEA for this example and Examples 2-4.

In a personal communication with the second author, Heredia-Langner indicated that the 12-point design reported in HCMBR was obtained from only a single computer run with a single setup of the GA. Hence, it is unknown whether additional runs with different GA setups may yield the same improved design obtained by FFEA.

Table 1. Four iterations of FFEA to improve a published 12-point design (points to be replaced by new ones are underlined).

x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2
<u>–1.0</u>	<u>1.0</u>	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0
–1.0	0.5	–1.0	0.5	<u>–1.0</u>	<u>0.5</u>	1.0	–1.0	1.0	–1.0
1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0
–1.0	1.0	–1.0	1.0	–1.0	1.0	–1.0	1.0	–1.0	1.0
–1.0	0.5	–1.0	0.5	–1.0	0.5	–1.0	0.5	–1.0	0.5
1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
0.5	–1.0	<u>0.5</u>	<u>–1.0</u>	–0.1	–0.4	<u>–0.1</u>	<u>–0.4</u>	–0.2	–0.3
0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
0.5	–1.0	0.5	–1.0	0.5	–1.0	0.5	–1.0	0.5	–1.0
1.0	–1.0	1.0	–1.0	1.0	–1.0	1.0	–1.0	1.0	–1.0

6.2. Example 2: Mixture Experiment with One Process Variable

Welch [21] described a mixture-process variable (MPV) experiment involving three mixture variables x_1, x_2, and x_3 and one process variable $x_4 \in \{-1, 0, 1\}$ using the model $E(y) = \Sigma_{i=1}^{3} \beta_i x_i + \Sigma_{i=1}^{3} \Sigma_{j=i+1}^{4} \beta_{ij} x_i x_j + \beta_{44} x_4^2$. The candidate set for this problem was a 273-point grid resulting from partitioning each mixture variable into 13 equally spaced levels (0, 1/ 12, …, 1) (yielding 91 mixtures) and then forming combinations with the process variable taking coded values of −1, 0, and 1 ($3 \times 91 = 273$). HCMBR obtained a 15-run design by the GA with $|\mathrm{X'X}|^{-1} = 0.3774$. They also reported a value of 0.5464 obtained by the MFEA.

We submitted the same candidate set and assumed model form to the FFEA, which produced a 15-run design (Table 2) with $|\mathrm{X'X}|^{-1} = 0.3750$, $v_{\max} = 0.9806$, and G-eff=68.0. For a problem of this size, there is little chance that the FFEA got trapped in local optima. We ran the FFEA 1000 tries (times), each try with a different starting design, and obtained designs with the mentioned value of $|\mathrm{X'X}|^{-1}$ 933 times. The cumulative distribution of $|\mathrm{X'X}|^{-1}$ for 1,000 FFEA-generated designs for Example 1 is given in Figure 1. Each try requires 4-10 iterations and about 500 (instead of $15 \times 273 = 4{,}095$) Fedorov delta functions are evaluated in each iteration. The total computer time spent for 1000 tries on the previously mentioned laptop was 15 seconds. The average number of successes per second for this example is therefore 62.2 (=933/ 15).

Table 2. 15-point MPV design.

x_1	x_2	x_3	x_4
0	0	1	−1
0	0	1	0
0	0	1	1
0	1/ 2	1/ 2	−1
0	1/ 2	1/ 2	1
0	7/ 12	5/ 12	0
0	1	0	−1
0	1	0	1
1/ 2	0	1/ 2	−1
1/ 2	0	1/ 2	1
1/ 2	1/ 2	0	−1
1/ 2	1/ 2	0	1
7/ 12	0	5/ 12	0
1	0	0	−1
1	0	0	1

6.3. Example 3: Gasoline Blending Mixture Experiment

Snee and Marquardt [19] described a gasoline blending experiment whose objective was to develop a blending model for a 5-component mixture experiment system. The five components were Butane (x_1), Alkylate (x_2), Lt. St. Run (x_3), Reformate (x_4) and Cat. Cracked (x_5), where $\Sigma x_i = 1$. The single-component constraints for the components were $0.00 \le x_1 \le 0.10$, $0.00 \le x_2 \le 0.10$, $0.05 \le x_3 \le 0.15$, $0.20 \le x_4 \le 0.40$ and $0.40 \le x_5 \le 0.60$. HCMBR used the GA to generate a 16-run D-optimal design for a linear mixture model $E(y) = \sum_{i=1}^{5} \beta_i x_i$ from a grid of step size 0.0001. The resulting design had $|\mathrm{X'X}|^{-1} = 13{,}827$. They also reported a design obtained using the MFEA with $|\mathrm{X'X}|^{-1} = 13{,}832$.

We applied the FFEA to this design problem using one of two candidate sets: (i) the 28 extreme vertices of the constrained region, and (ii) the 22,041 points on a grid of step size 0.01 that satisfied the single-component constraints. For both candidate sets, the FFEA found the same best design (Table 3) with $|X'X|^{-1}=13{,}808$, $v_{\max}=0.3346$, and G-eff=93.4. This value of $|X'X|^{-1}$ appears in 15 out of 1000 tries using the first candidate set and 21 out of 1000 tries using the second candidate set (Figure 1). The FFEA used 1.3 seconds for 1000 tries with the first candidate set and about 4 minutes with the second candidate set. The average number of successes per second for this example is therefore 11.5 (=15/ 1.3) for the first candidate set and 0.0875 (=21/ 240) for the second candidate set.

Table 3. Mixture design for the gasoline blending experiment.

x_1	x_2	x_3	x_4	x_5
0.0	0.00	0.05	0.35	0.60
0.0	0.00	0.05	0.35	0.60
0.0	0.00	0.05	0.35	0.60
0.0	0.05	0.15	0.40	0.40
0.0	0.10	0.05	0.40	0.45
0.0	0.10	0.15	0.20	0.55
0.0	0.10	0.15	0.20	0.55
0.0	0.10	0.15	0.35	0.40
0.1	0.00	0.10	0.40	0.40
0.1	0.00	0.15	0.20	0.55
0.1	0.00	0.15	0.20	0.55
0.1	0.00	0.15	0.35	0.40
0.1	0.10	0.05	0.20	0.55
0.1	0.10	0.05	0.20	0.55
0.1	0.10	0.05	0.35	0.40
0.1	0.10	0.05	0.35	0.40

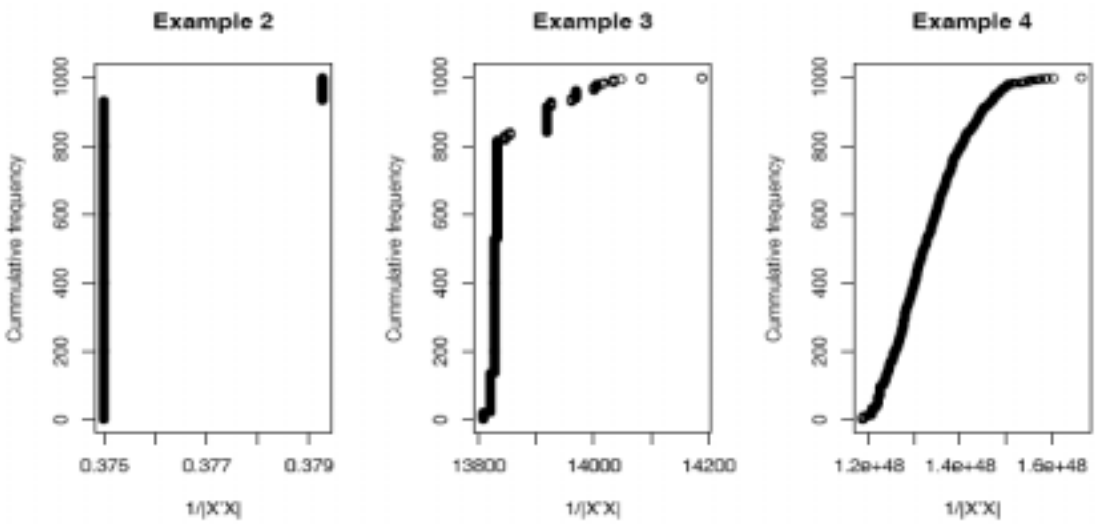

Figure 1. Cumulative distributions of $|X'X|^{-1}$ from 1000 FFEA-generated designs for Examples 2, 3 and 4 (each point on a graph represents the result of at least one try).

6.4. Example 4: Plastic Formulation Mixture Experiment

Snee [20] described a plastic formulation mixture experiment whose objective was to evaluate the effects of five components on the hardness of the resulting plastic product. The five components were: binder (x_1), co-binder (x_2), plasticizer (x_3), monomer A (x_4), and monomer B(x_5), where $\Sigma x_i = 1$. The single-component constraints were, $0.50 \le x_1 \le 0.70$, $0.05 \le x_2 \le 0.15$, $0.05 \le x_3 \le 0.15$, $0.10 \le x_4 \le 0.25$, and $0.00 \le x_5 \le 0.15$, while the multi-component constraints were $0.18 \le x_4 + x_5 \le 0.26$ and $x_3 + x_4 + x_5 \le 0.35$. HCMBR started with a grid of step size 0.0001, and applied a GA to obtain a 25-run D-optimal design for a quadratic mixture model $E(y) = \Sigma_{i=1}^{5} \beta_i x_i + \Sigma_{i=1}^{4} \Sigma_{j=i+1}^{5} \beta_{ij} x_i x_j$. The resulting design had $|X'X|^{-1} = 1.217E48$. They also reported a design obtained using the MFEA with $|X'X|^{-1} = 1.256E48$.

We gave the FFEA a 10,468-point candidate set (consisting of those points in a grid of step size 0.01 that satisfied the mentioned single- and multi-component constraints) and 1000 tries to work on this problem. The FFEA found a design (Table 4) with $|X'X|^{-1} = 1.187E48$, $v_{max} = 0.7811$, and G-eff=76.8, which was achieved six times out of 1000 tries (Figure 1). These 1000 tries required 18 minutes. The average number of successes for this example is therefore 1/ 3 (=6/ 18) per minute or 20 per hour.

Table 4. Mixture design for the plastic formulation experiment.

x_1	x_2	x_3	x_4	x_5
0.50	0.15	0.09	0.11	0.15
0.50	0.15	0.09	0.25	0.01
0.50	0.15	0.15	0.10	0.10
0.50	0.15	0.15	0.20	0.00
0.54	0.15	0.05	0.18	0.08
0.55	0.15	0.05	0.10	0.15
0.56	0.09	0.10	0.10	0.15
0.56	0.11	0.15	0.18	0.00
0.56	0.15	0.11	0.10	0.08
0.58	0.15	0.05	0.22	0.00
0.59	0.10	0.05	0.25	0.01
0.59	0.10	0.09	0.16	0.06
0.60	0.05	0.09	0.18	0.08
0.60	0.05	0.10	0.25	0.00
0.60	0.05	0.15	0.10	0.10
0.60	0.05	0.15	0.20	0.00
0.62	0.05	0.15	0.10	0.08
0.62	0.15	0.05	0.10	0.08
0.62	0.15	0.05	0.18	0.00
0.64	0.05	0.05	0.11	0.15
0.65	0.05	0.05	0.25	0.00
0.67	0.05	0.10	0.18	0.00
0.69	0.05	0.05	0.10	0.11
0.70	0.07	0.05	0.10	0.08
0.70	0.07	0.05	0.18	0.00

To get a fair idea of the difference in performance between the FEA and its approximations, we gave the design problems in Examples 1-4 to ACED (software implementing an approximation of the FEA mentioned in Section 3). While ACED obtained FFEA results for Examples 1 and 2 very quickly, it failed to match FFEA results for examples 3 and 4 after 1000 tries.

6.5. Example 5: Grout Component-Amount Experiment

Piepel *et al.* [17] reported an example involving four dry blend materials used to make grout from low-level nuclear waste: cement (x_1), flyash (x_2), attapulgite clay (x_3) and slag (x_4), where the levels of each are expressed in pounds per gallon of waste. The experimental region is defined by the following constraints: $0.5 \le x_1 \le 3.5$, $0.0 \le x_2 \le 6.0$, $0.5 \le x_3 \le 2.0$, $0.0 \le x_4 \le 6.0$, $1.5 \le x_1 + x_2 \le 7.5$, and $6.0 \le \sum x_i \le 10.0$. Note that the x_i are amounts and not proportions of the dry-blend ingredients, so this is a constrained component-amount (rather than mixture) experiment.

Piepel *et al.* [17] assumed a second-order polynomial model and generated designs with $n = 20$, 25 and 30 points using several of the optimality criteria available in ACED. They used a candidate set consisting of: (i) the 31 vertices, 63 one-, 44 two-, and 12 three-dimensional face centroids of the constrained experimental region, (ii) 0.8, 0.6, 0.4, and 0.2 shrunken (toward the center point) versions of these 150 points, and (iii) the center point of the region. Hence, they supplied total of 751 candidate points to ACED. Because of computing power limitations in 1993, they performed only 30 tries with each optimality criterion.

ACED using both the G- and D-optimality criteria and the FFEA were run with 1000 tries, the same model, and a larger 2,277-point candidate set to construct designs containing $n = 20$, 25, and 30 points. This larger candidate set was formed with a grid of step size 0.5, and retaining those points satisfying the previously described constraints. Table 5 lists the properties of (i) the G-optimal designs reported in Piepel *et al.* [17], (ii) the best G-optimal designs out of the 1000 ACED G-optimal designs, (iii) the best G-optimal designs out of the 1000 ACED D-optimal designs, and (iv) the best G-optimal designs out of the 1000 FFEA D-optimal designs.

While it is not obvious for $n = 30$, it is clear for $n = 20$ and 25 that FFEA designs are better than ACED designs with respect to G- and D-optimality. This result supports our strategy of constructing G-optimal designs, i.e. selecting the best G-optimal designs from a large pool of D-optimal designs. As expected, all new designs in Table 5 are notably better than the corresponding designs in Piepel *et al.* [17] with respect to the reported properties, because more tries and a larger candidate set (which contains more boundary points) were used. The distributions of $v_{\max}$ for FFEA designs for $n = 20$, 25 and 30 are given in Figure 2.

Each 1000 tries of the FFEA for each n consumed about 4 minutes on the 2GHz laptop previously mentioned, and about 2.5 minutes on a 3GHz PC. Each 1000 tries of ACED for each n consumed about 2 minutes on a 3GHz PC when G-optimality was used and 1 minute on this PC when D-optimality was used. Note that we implemented the FFEA in Java, which is an interpreted language. Therefore, a C++ or Fortran (the language used to write ACED) implementation of the FFEA is expected to be up to five times faster than a Java implementation of this algorithm on a comparable computing platform. Also note that the implementation of G-optimality in ACED is the generalization of the DETMAX algorithm (Welch [21]), an approximation of the FEA that includes some of the same improvements included in the FFEA. These reasons explain the impressive speed of the ACED implementation.

Table 5. Properties of designs for grout experiment.

n	Criterion	By	$v_{\max}$	G-eff	$\overline{v}$	$\lvert X'X\rvert^{-1/p}$
20	G	ACED*	1.041**	72.0	0.646**	0.0327
	G	ACED	0.968	77.5	0.622	0.0331
	D***	ACED	0.995	75.4	0.666	0.0328
	D***	FFEA	0.957	78.4	0.626	0.0327
25	G	ACED*	0.797**	75.2	0.535**	0.0261
	G	ACED	0.745	80.6	0.512	0.0262
	D***	ACED	0.764	78.5	0.501	0.0261
	D***	FFEA	0.736	81.5	0.512	0.0256
30	G	ACED*	0.604**	82.6	0.412**	0.0215
	G	ACED	0.591	84.6	0.426	0.0214
	D***	ACED	0.591	84.6	0.408	0.0211
	D***	FFEA	0.587	85.1	0.417	0.0213

*Only 30 tries (instead of 1000 tries) were used (Piepel *et al.* [17]).
**Calculated over a 751-point grid instead of a 2,277-point grid.
***D criterion was used but the best G-optimal design was selected.

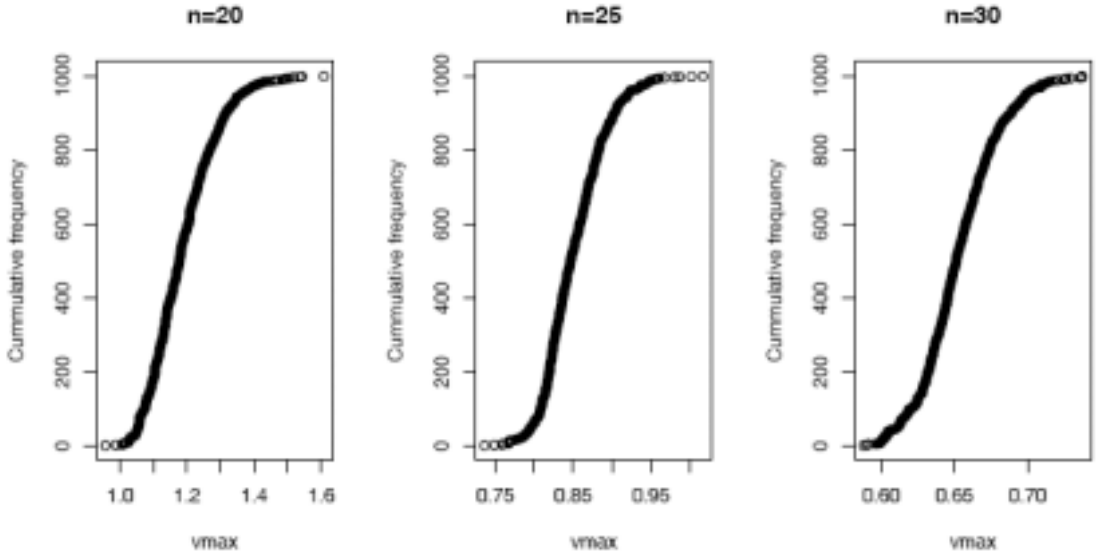

Figure 2. Cumulative distributions of $v_{\max}$ from 1000 FFEA-generated designs for Example 5 (each point on a graph represents the result of at least one try).

7. Concluding Remarks

This paper reviewed the FEA, other PEAs commonly in use, and presented a faster implementation of the FEA referred to as the fast-FEA (denoted FFEA). The FFEA was applied to several constrained region examples from the literature to provide benchmark results on the success rates in obtaining the best D-optimal designs and the computer time used. The results for the examples show the FFEA improves on D-optimal designs obtained by other algorithms such as the MFEA, generalized DETMAX, and GA.

Despite these results, we believe that no-candidate-set algorithms such as the GA and CEAs (Meyer and Nachtsheim [13]; Nguyen [14]; Piepel *et al.* [18]) have a role to play. These algorithms have the potential to work for very large constrained mixture and other design problems where it is impossible to use the candidate-set-based approach (see Piepel *et al.* [18]). However, no-candidate-set algorithms are still at the infancy stage of development. Better and faster implementations of these algorithms will surely one day catch up with existing PEAs requiring candidate points. However, even when that time comes, there will still be situations (e.g., when the design must be constructed from a specific set of candidate points) where a candidate-set-based PEA will be preferred. Hence, it is important that high-quality, fast PEAs such as the FFEA be available and implemented in software.

The FFEA is implemented in a program called FEADO (Fedorov Exchange Algorithm for constructing D-Optimal experimental designs). More examples of D-optimal designs constructed by FEADO can be found at http://designcomputing.net/feado. The Java byte code of this program is available from the first author upon request.

Finally, we recommend that in constructing CGDs using a PEA such as the FFEA, a large number of tries (e.g., 1000) be conducted using a sufficiently large candidate set. The traditional practice of making 10-30 tries does not appear to be sufficient to identify the best designs in some examples. Further, the approach of selecting the best G-optimal design out of a large number of D-optimal tries is recommended as yielding G-optimal designs with properties similar to or better than those obtained using a G-optimality criterion. Many commercial software packages with optimal design capability implement only the D-optimality criterion, so this approach provides for obtaining very good G-optimal designs with such software.

Acknowledgements

The first author dedicates this paper to Alan J. Miller, a wonderful colleague, co-author, and friend. We would like to thank the Editor and two referees for valuable comments and suggestions that enhanced the content and readability of the paper. Our thanks are also extended to Pat Whitcomb (StatEase, Inc.) for comments on the first version of the paper.

References

1. Cook, R. D. and Nachtsheim, C. J. (1980). A comparison of algorithms for constructing exact D-optimal designs. *Technometrics*, 22, 315-324.
2. Fedorov, V. V. (1969). *Theory of Optimal Experiments*. Preprint No. 7 LSM, Izd-vo Moscow State University, Moscow, USSR.
3. Fedorov, V. V. (1972). *Theory of Optimal Experiments*. Trans. and ed. by W. J. Studden and E. M. Klimko. New York, Academic Press.
4. Galil, Z. and Kiefer J. (1980). Time- and space-saving computer methods, related to Mitchell's DETMAX for finding D-optimal designs. *Technometrics*, 22, 301-313.
5. Hardin, R. H. and Sloane, N. J. A. (1993). A new approach to the construction of optimal designs. *Journal of Statistical Planning & Inference*, 37, 339-369.
6. Heredia-Langner, A., Carlyle, W. M., Mongomery, D. C., Borror and C. M., Runger, G.C. (2003). Genetic algorithm for the construction of D-optimal designs. *Journal of Quality Technology*, 35, 28-46.
7. Miller A. J. and Nguyen, N-K. (1994). A Fedorov exchange algorithm for D-optimal

designs. *Applied Statistics*, 43, 669-678.

8. Mitchell, T. J. (1974a). An algorithm for the construction of D-optimal designs. *Technometrics*, 16, 203-210.
9. Mitchell, T. J. (1974b). Computer construction of "D-optimal" first-order designs. *Technometrics*, 16, 211-220.
10. Mitchell, T. J. and Miller, F. L., Jr. (1970). Use of "design repairs" to construct designs for special linear models. *Mathematics Division Annual Progress Report* (ORNL-4661), Oak Ridge National Laboratory, Oak Ridge, Tennessee, 130-131.
11. Montgomey, D. C. (2001). *Design and Analysis of Experiments*, 5th edition. John Wiley, New York.
12. Montgomery, D. C., Loredo, E. N., Jearkpaporn D. and Testik, M. C. (2002). Experimental designs for constrained regions. *Quality Engineering*, 14, 587-601.
13. Meyer, R. K. and Nachtsheim, C. J. (1995). The coordinate exchange algorithm for constructing exact optimal designs. *Technometrics*, 37, 60-69.
14. Nguyen, N-K. (2002). A modified cyclic-coordinate exchange algorithm as illustrated by the construction of minimum-point second-order designs. *Advances in Statistics, Combinatorics and Related Areas*. Edited by C. Gulati, Y-X Lin, S.Mishra, J. Rayner. World Scientific Publishing Co. Pte. Ltd., 205-210.
15. Nguyen, N-K. and Miller A. J. (1992). A review of some exchange algorithms for constructing discrete D-optimal designs. *Computational Statist. & Data Analysis*, 14, 489-498.
16. Nguyen, N-K. and Miller A. J. (1996). 2^m fractional factorial designs of resolution V with high A-efficiency, $7 \le m \le 10$. *Journal of Statistical Planning & Inference,* 59, 379-384.
17. Piepel, G. F., Anderson C. M. and Redgate P. E. (1993). Response surface designs for irregularly-shaped regions. *1993 Proceedings of the Section on Physical and Engineering Sciences*, 205-227, American Statistical Association, Alexandria, Virginia.
18. Piepel, G. F., Cooley, S. K. and Jones, B. (2005). Construction of a 21-component layered mixture experiment design using a new mixture coordinate-exchange algorithm. To appear in *Quality Engineering*.
19. Snee, R. D. and Marquardt, D. W. (1974). Extreme vertices designs for linear mixture models. *Technometrics*, 16, 399-408.
20. Snee, R. D. (1985). Computer-aided design of experiments–some practical experiences. *Journal of Quality Technology*, 17, 222-236.
21. Welch, W. J. (1984). Computer-aided design of experiments for response estimation. *Technometrics*, 26, 217-224.
22. Welch, W. J. (1987). *ACED, Algorithms for the construction of experimental designs, Users guide version 1.6.1.* University of Waterloo, Waterloo, Ontario, Canada.
23. Wynn, H. P. (1972). Results in the theory and construction of D-optimum experimental designs. *Journal of the Royal Statistical Society*, B, 34, 133-147.

Authors' Biographies:

Nam-Ky Nguyen (http://turing.une.edu.au/nkn) received his Ph.D. in Agricultural Statistics at the Indian Agricultural Statistics Research Institute under Dr. Aloke Dey. He is currently a Senior Lecturer in the School of Mathematics, Statistics & Computer Science, University of New England, Australia. He is also the developer of the Gendex DOE toolkit (http://designcomputing.net/gendex). This toolkit is currently in use at more than 50

universities and research organizations worldwide. He has been working extensively in the area of computer-generated designs. He has about 30 publications in applied statistics / computing and collaborative research.

Greg Piepel received his Ph.D. in Statistics at the University of Florida and is a Laboratory Fellow in the Statistical Sciences group at Battelle-Pacific Northwest Division in Richland, Washington, USA. He is also the developer of the MIXSOFT software and presents short courses on the design and analysis of mixture experiments (http:// members. aol.com/ mixsoft). His research interests are in the design and analysis of mixture and other constrained region experiments, optimal experimental design, statistical methods development, and solving applied problems in the physical and engineering sciences. Dr. Piepel is a Fellow of the American Statistical Association and is on the Editorial Review Board of the *Journal of Quality Technology*. He has published papers in *Technometrics*, *Journal of Quality Technology*, *The American Statistician*, *Stats*, *Quality Engineering*, *Journal of the American Ceramic Society*, *Journal of Non-Crystalline Solids*, and several other journals.